

Letters to the Editor

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PRELIMINARY REPORT ON THE CRYSTAL STRUCTURE OF ANTHRONE

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The crystal structure of Anthrone is determined by means of two dimensional Fourier Synthesis in the 010 plane. This plane is chosen as the molecule is well resolved in projection on this plane according to the trial structure. The space group of anthrone together with other crystallographic data has already been published by Srivastava (1957). However the axial lengths were again determined with the values of Bragg angles, obtained after correcting them for film shrinkage errors by the author's method (Srivastava, 1959). The revised values thus obtained are

$a = 15.80 \text{ \AA}; \quad b = 3.998 \text{ \AA}; \quad c = 7.86 \text{ \AA}.$ The space group being $P2_1/a-C_{2h}^5$.

The values of the atomic coordinates which were obtained after the third refinement of F_0 synthesis are given in the table, taking the X and Z coordinates from the projection, and deriving the y coordinates from the standard inter-atomic distances. The value of the reliability index

$$R = \frac{\sum |F_0| - \sum |F_c|}{\sum |F_0|}$$

came out to be 0.267.

(The symbol 0 refers to the Oxygen atom and all other letters refer to carbon atoms.)

TABLE I

| Atom | X in AU | Y in AU | Z in AU |
|------|---------|---------|---------|
| A' | 2.12 | 3.65 | 3.10 |
| B' | 0.89 | 3.08 | 2.67 |
| C' | 0.44 | 2.56 | 1.34 |
| E | 1.33 | 2.60 | 0.46 |
| F | 2.65 | 3.18 | 0.89 |
| G | 3.08 | 3.70 | 2.14 |
| D | 0.98 | 2.05 | -0.93 |
| O | 1.70 | 2.09 | -1.61 |
| A | -2.12 | 0.35 | -3.10 |
| B | -0.89 | 0.92 | -2.67 |
| C | -0.44 | 1.44 | -1.34 |
| E' | -1.33 | 1.40 | -0.46 |
| F' | -2.65 | 0.82 | -0.89 |
| G' | -3.08 | 0.30 | -2.14 |
| D' | -0.98 | 1.95 | 0.93 |

The molecule is assumed to be planar, and the origin is chosen at the centre of symmetry. The atomic scattering factors for carbon atoms were taken as

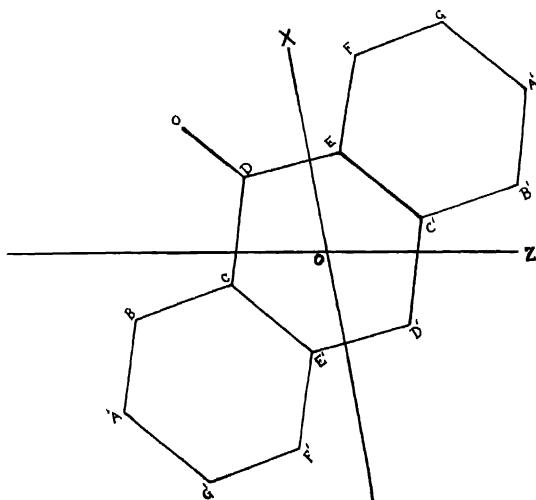


Fig. 1.

those for the general carbon atom for the anthraquinone, and for oxygen atom as that taken in the case of oxygen of anthraquinone by Murty (1957), since the

two structures are strikingly very similar. Refinement of the structure by the Difference Synthesis is in progress.

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ON THE CRYSTAL STRUCTURE OF METHANOL AT -180°C

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The crystal structure of methanol has been studied by Tauer and Lipscomb (1952) by studying the Weissenberg and precession photographs of the crystal at -110°C and at -160°C . They reported that the crystal has a transition at -115°C the high temperature modification being orthorhombic conforming to the space group D_{2h}^{17} . The Weissenberg photographs taken for the crystal at -160°C show that the low temperature phase consists of small crystallites of low symmetry but not of a single crystal. They observed that the possible unit cell which accounts for all but a few weak reflections is monoclinic with two molecules in the unit cell having dimensions $a = 4.53 \text{ A.U.}$, $b = 4.69 \text{ A.U.}$, $c = 4.91 \text{ A.U.}$ and $\beta = 90^{\circ} \pm 3^{\circ}$. The space group C_{2h}^{28} was assigned to the crystal although they suggested the presence of some weak reflections indicating a super lattice. An attempt has been made to find out whether the crystal retains this symmetry at still lower temperatures upto -180°C .

The Debye-Scherrer pattern due to the crystal at -180°C was photographed by the method used earlier (Krishna Murti and Sen, 1956). The spacings calculated from the pattern obtained for the crystal at -180°C are given in Table I. The pattern has been analysed by trial and error method and it has been found that the crystal is monoclinic with the unit cell dimensions as $a = 4.59 \text{ A.U.}$, $b = 4.68 \text{ A.U.}$, $c = 4.92 \text{ A.U.}$ and $\beta = 97^{\circ}30'$. The density of the crystal at -180°C